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Microstructure Evolution in Irradiated Materials

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DISCLAIMER

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Project title: Microstructure evolution in irradiated materials

Research Objectives:
Study the interaction of defects produced during irradiation or deformation of a metal with the microstructure of that particular material, such as dislocations and grain boundaries. In particular we will study the interaction of dislocation with interstitial loops and stacking fault tetrahedral, and the production of displacement cascades close to dislocations and grain boundaries. The data obtained from these simulations will be used as input to diffusion models and dislocation dynamics models.

Significance of Research:
The interaction of defects produced during irradiation with the microstructure is responsible for material degradation under irradiation. Fundamental studies of the interaction of defects with dislocations and grain boundaries are necessary to develop predictive models for materials performance under irradiation and deformation, important issues in the development of materials for fusion reactors, as an example.

Computations Approach:
Mostly we will employ molecular dynamics simulations using empirical interatomic potentials. Parinello-Rahman boundary conditions will be used to apply stress to study dislocation motion. The link cell method is used to efficiently calculate the neighbors of the atoms in the computational box. The partition into link cells is also used to distribute the atoms across the nodes in the parallel machine. This code is written in Fortran and both MPI and PVM versions for message passing are available.

Study of defect diffusion is done using kinetic Monte Carlo models. The reactions rates for defect interaction and defect dissolution are input for this method, as well as the defect distribution, obtained from molecular dynamics simulations. Only a serial version of this code is available at the moment. This code is written in C.

Accomplishments
Study of the formation of a stacking fault tetrahedral (SFT) in copper both from the collapse of a vacancy plane and directly during irradiation. The presence of SFT after irradiation of copper has been observed experimentally for many years, however molecular dynamics simulations have failed until now to reproduce this observations. We have been able to simulate the production of a SFT during irradiation of copper by using high energy irradiation and long relaxation times.

Systematic study of damage produced by self-irradiation of copper, for energies between 200eB up to 20keV. Several cascades were obtained for each energy (maximum 12 and minimum 5A). The defect production as a function of energy was compared to that obtained from the Kinchin-Pease model. The

production rate is comparable to the Kinchin-Pease only for low energies, reaching a constant value of 0.2xKinchin-Pease at energies ~ 5keB. The data base extracted from this simulations was used to study defect accumulation and diffusion using kinetic Monte Carlo. One of the cascades was followed for 100ps. An interstitial cluster containing 38 defects was produced in this cascade. This interstitial is highly mobile and its migration is followed in this simulation. The next step in our simulations is to study the interaction of these type of clusters with dislocations.

Relevant Publications.

M.J. Caturla, N. Soneda, E. Alonso, B. Wirth, T., Diaz de la Rubia, J.M Perlado, Comparative study of radiation damage accumulation in Cu and Fe, submitted to J. Nucl. Mater.

E. Alonso, M.J. Caturla, T. Diaz de la Rubia, J. M. Perlado, Simulation of damage production and accumulation in vanadium, submitted to J. Nucl. Mater.

N. Soneda, T. Diaz de la Rubia,
Defect production, annealing kinetics and damage evolution in alpha-Fe: an atomic-scale computer simulation
Philosophical Magazine A. Vol. 1998, vole. 78, 995

W.J. Weber, R.C. Ewing, C.R.A. Catlow, T. Diaz de la Rubia
Radiation effects in crystalline ceramics for the immobilization of high-level nuclear waste and plutonium
Journal of Materials Research, June 1998, col. 13, 1434-84

R. Devanathan, W.J. Weber, T. Diaz de la Rubia
Computer simulation of a 10keV Si displacement cascade in SiC
Nuclear Instruments and Methods B, 1998, 141, 118

K. Nordlund, M. Ghaly, R. S. Averback, M. J. Caturla, T. Diaz de la Rubia
Defect production in collision cascades in elemental semiconductors and fcc metals
Physical Review B, 1998, vol. 57, 7556

R. Devanathan, T. Diaz de la Rubia, W. J. Weber,
Displacement threshold energies in beta SiC
Journal of Nuclear Materials, 1998, vol. 253 47

R. Diaz de la Rubia, N. Soneda, M.J. Caturla, E. Alonso,
Defect production and annealing kinetics in elemental metals and semiconductors
Journal of Nuclear Materials, 1997, vol. 251

T. Diaz de la Rubia. J.M. Perlado, M. Tobin,
Radiation effects in silicon carbide: high energy cascades and damage accumulation at high temperature
Journal of Nuclear Materials 1996, 233-237B, 1096

Justification for Resources Requested:
A typical simulation of the interaction of a dislocation with a defect requires a minimum of 1 million atoms, and a total number of 30,000 to 60,000 steps. Each time step on 64 nodes of a Cray T3E requires 1 second of CPU per million atoms. That is, between 8 and 16 CPU hours are necessary for a single case using 64pe, or a total of 16x64 1,000 node hours. A complete data base for different defects types (vacancies and interstitials of different sizes) and different energies for the cascades is necessary. Specifically we want to study the inte4raction of SFT, interstitial loops, vacancy loops and cascades with dislocations plus the interaction of cascades with grain boundaries, a minimum of 10-15 cases for each is necessary, that is a total time between 50 and 75,000 node hours.

Each run generates of the order of 0.5 Gbytes of storage, although not all has to be kept for long ties, only about 0.1 Gbytes per run.

Most of the time will be used for production, however, a small part will be used to develop new subroutines for output and boundary conditions.

In addition, we expect to de extensive kinetic Monte Carlo calculation on the J90 of damage evolution and defect kinetics. These require about 10 hours of CPU for realistic damage doses to evolve the system microstructure to macroscopic times of the order of tens on thousands of seconds of real time.

Code descriptions:
The MDCASK does is written in Fortran, and uses MPI for message passing. A PVM version of the code also exists. The link cell method for calculation of neighbors of the atoms in the simulation is used. The link cell decomposition is used for parallelization. The code scales linearly with the number of nosed with the computational box is sufficiently big.

Development of the code will focus in new subroutines for output: parallel I/O, as well as new methods of sorting the important output to write into a file, since, as the number of atoms increases, the selection of the relevant output becomes critical. Memory optimization and selection of the number of nodes as an external variable are also planed for code development.

Figures representative of the work:

Figure 1:
Damage produced by a 20keV recoil atom in Copper. The red spheres represent the location of interstitial atoms, the green spheres represent vacancy sites. The simulation was done using 500,000 atoms for a total time of 35 ps, or approximately 45,000 steps, using 64 processors, and a performance of ~2s per time step. The damage produced in this fcc material due to irradiation results in large clusters of interstitials and vacancies. The production of a large interstitial cluster that migrates along a <110> direction is observed in this simulation.

The graphics were obtained using Renderman on a Silicon Graphics, as a tiff file, and then edited to add titles in AdobePhotoshop on a Macintosh.

Figure 2:
Damage produced by a 50keV recoil atom in Tungsten. The red spheres represent the location of interstitial atoms, the green spheres represent vacancy sites. The simulation was done using 1,458,000 atoms for a total time of 35 ps, or approximately 8,000 steps, using 64 processors, and a performance of ~1.6s per time step. Unlike the case of Cu, where large clusters of vacancies and interstitials are formed, the damage produced in this bcc material is mainly isolated vacancies and some clusters of interstitials. This simulation clearly shows the break up into subcascades, and the production of two smaller cascades.

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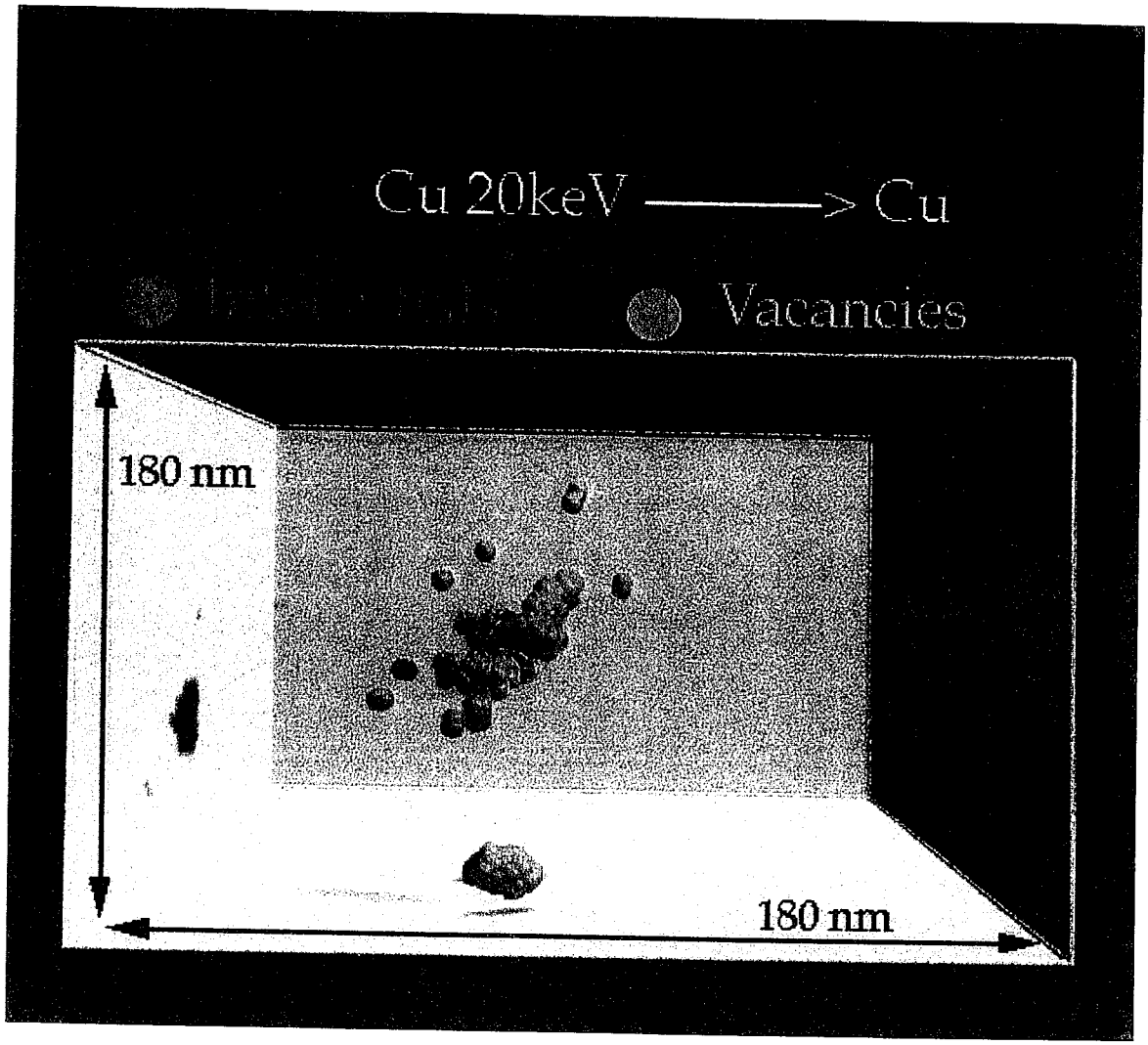
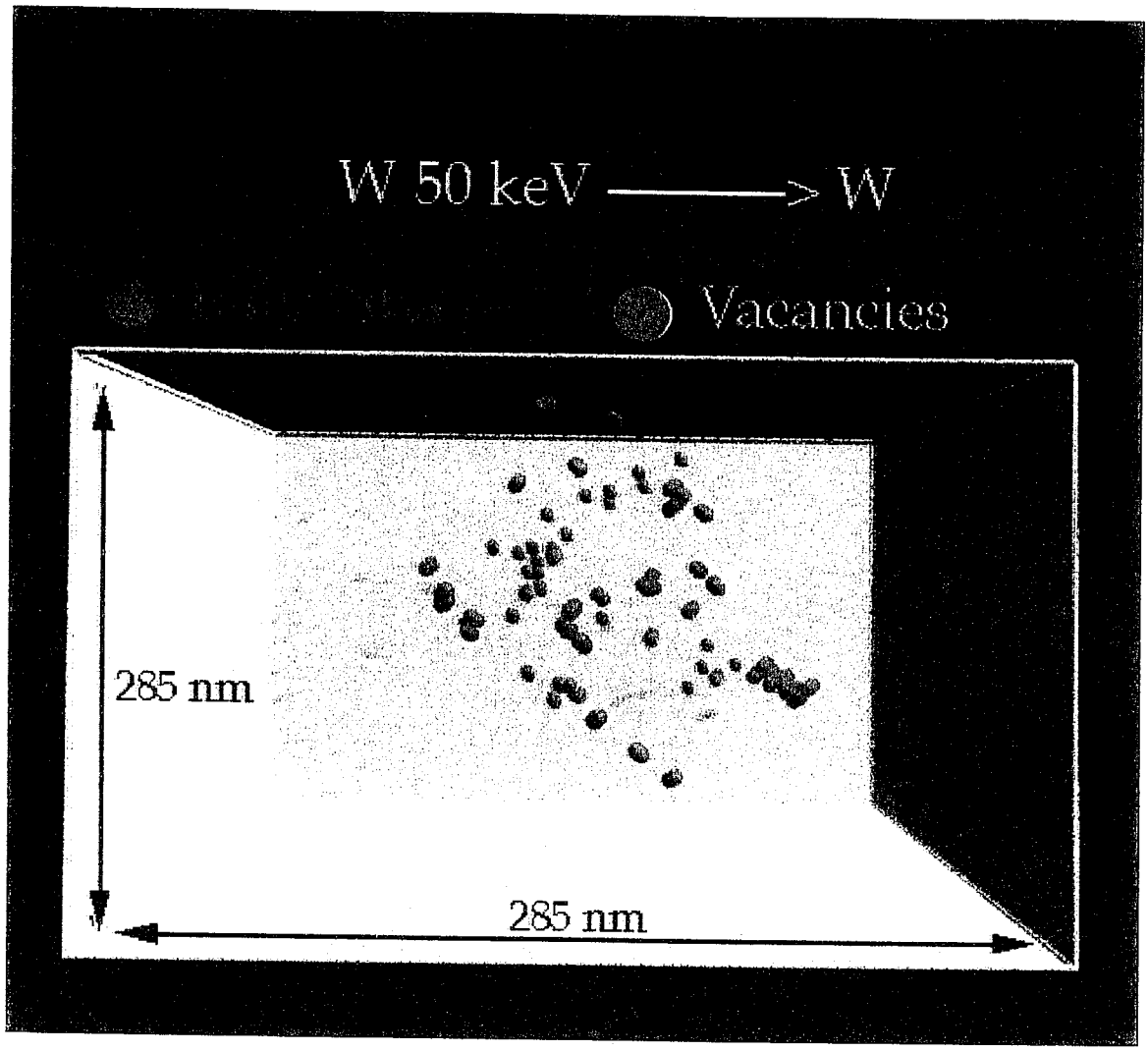

Cu 20keV ——> Cu
Vacancies
180 nm
180 nm


W 50 keV ——> W
Vacancies
285 nm
285 nm

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